

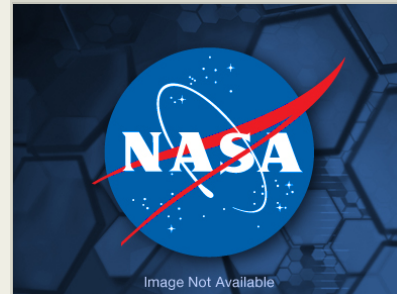
Computational Studies of Inelastic Scattering using Mixed Quantum/Classical Theory

Completed Technology Project (2017 - 2019)



Project Introduction

Molecules are an important component of the universe that dominates the cooling process and determines the degree of ionization of interstellar gas clouds and, hence, regulates star and planet formation. The exploration of paths toward chemical complexity in space has direct bearing on the origin and evolution of life. Moreover, molecular transitions provide a sensitive probe of the dynamics and the physical and chemical conditions in a wide range of objects at scales ranging from newly forming planetary systems to galactic and extragalactic sizes. In the vast majority of the conditions present in the interstellar/circumstellar/cometary media, the so-called collisional de-excitation rate coefficients are indispensable to convert an observed signal into a species column density and, therefore, abundance, and to constrain the density and temperature of the emitting or absorbing gas. However, a significant part of this information is still missing and there is no simple way of determining it from the laboratory experiments. In order to fill this serious gap, we will approach the problem by employing a mixture of quantum and classical mechanics in a state-of-the-art theoretical approach to the dynamics of molecule + quencher collision. We showed that it is feasible to simplify the physical model and gain a significant computational advantage by treating selected degrees of freedom classically, while the most important internal degrees of freedom are still treated quantum mechanically. In this project we propose to carry out: i) Benchmark MQCT calculations of rotational quenching of H₂O (including deuterated forms) by H₂ at lower temperatures first, to compare against the existing full-quantum scattering calculations, but then at higher temperatures where no accurate data exists, up to , typical to hot cores and corinos, outflow shocks, and the innermost regions of protoplanetary discs. ii) Conceptually new calculations of ro-vibrational quenching and excitation of the most astronomically relevant excited bending mode of H₂O, first by atomic quencher, He, and then by molecular quencher, H₂, using MQCT, in a broad range of temperatures, up to when these processes become important (typical to red supergiant stars). iii) First detailed calculations for H₂O + H₂O rotational quenching and excitation within MQCT framework in the temperature range relevant to warm star-forming regions or cometary environment. Deuterated forms of ortho/para-water can all be studied.



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Organizational Responsibility

Responsible Mission Directorate:

Science Mission Directorate (SMD)

Responsible Program:

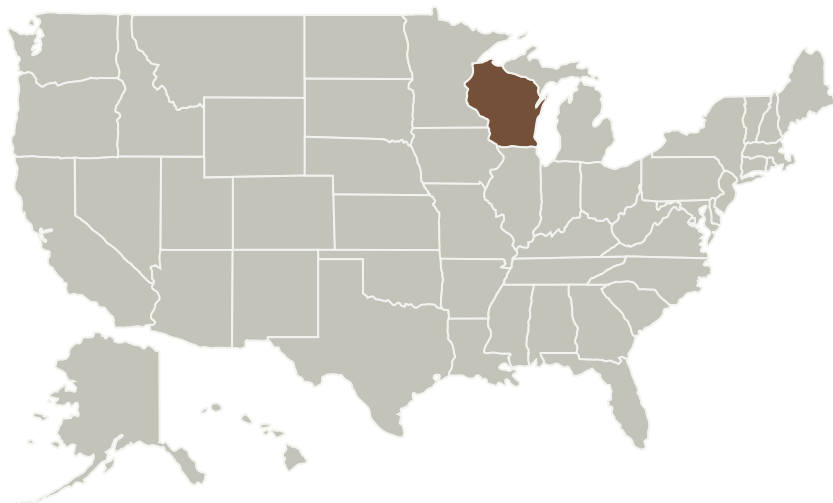
Astrophysics Research and Analysis

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Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
Marquette University	Supporting Organization	Academia	Milwaukee, Wisconsin

Primary U.S. Work Locations

Wisconsin

Project Management

Program Director:

Michael A Garcia

Program Manager:

Dominic J Benford

Principal Investigator:

Dmitri Babikov

Co-Investigator:

Katherine Durben

Technology Areas

Primary:

- TX01 Propulsion Systems
 - └ TX01.3 Aero Propulsion
 - └ TX01.3.6 Ramjet/Scramjet

Target Destination

Outside the Solar System